

Brownian motion in fluctuating periodic potentials

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Abstract

This work deals with the overdamped motion of a particle in a fluctuating one-dimensional periodic potential. If the potential has no inversion symmetry and its fluctuations are asymmetric and correlated in time, a net flow can be generated at finite temperatures. We present results for the stationary current for the case of a piecewise linear potential, especially for potentials being close to the case with inversion symmetry. The aim is to study the stationary current as a function of the potential. Depending on the form of the potential, the current changes sign once or even twice as a function of the correlation time of the potential fluctuations. To explain these current reversals, several mechanisms are proposed. Finally, we discuss to what extent the model is useful to understand the motion of biomolecular motors.

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1 Introduction

Protein motors play an important role in intracellular transport phenomena. In the cytoplasm of eucaryotic cells, certain macromolecules move along a complex network of periodic polymer tracks and transport organelles or vesicles containing chemicals. These ATP-hydrolysing macromolecules successively attach to and detach from the biopolymer while walking on it. Structural analysis of several motor proteins together with *in vitro* experiments have revealed that they undergo a cyclic sequence of conformational changes to convert the chemical energy from the ATP-hydrolysis into a unidirectional movement along the biopolymer. (see [1] and the references therein). Although this mechanochemical conversion mechanism is not yet fully understood, there is no macroscopic thermal or chemical gradient in the cell medium that determines the direction of movement. Thus an interesting question arises: which properties of the system *protein+track* favour one direction of movement rather than the opposite? This is certainly a difficult matter: one knows motor proteins of the same family that move in different directions along the same track.

Recently, some progress has been made in attempting to answer the above question. Apparently, the biasing of the catalytic cycle of the ATP hydrolysis is due to time-correlated chemical fluctuations induced by far-from-equilibrium concentrations of the reactants. To describe the motion of molecular motors, Magnasco considered the model of a Brownian particle moving in a one-dimensional ratchet-like potential driven by a symmetric stochastic force [2]. A similar model has been used by Feynman *et al.* [3] to illustrate the Second Law of Thermodynamics: Thermal fluctuations cannot produce a transport. (The example is originally due to Smoluchowski [4].) But if the fluctuations of the force are time-correlated, the restrictions of the Second Law of Thermodynamics cease to apply and the particle shows a net movement that can even overcome the action of an external force: The asymmetric ratchet works as a mechanical rectifier. Both ingredients, the time correlation of the symmetric fluctuations and the lack of inversion symmetry of the potential yield a non vanishing current.

Astumian and Bier [5] proposed a different picture for the motion of motor proteins. They studied the problem of a strongly damped particle moving in a ratchet-like potential that fluctuates dichotomously, i.e. between two different states [5]. The two different states of the potential model the electrostatic interaction of the motor protein with the periodic charge pattern of the biopolymer. The charge of the protein is changed when ATP binds to it. As a result, the potential changes as well. In this model, a net current is obtained at finite temperatures if the coloured potential fluctuations are asymmetric. Similar models have also been proposed by Prost *et al.* [6, 7]. These authors argued that the two states correspond to the attached and the detached state of the motor protein. For a recent overview on this and related models we refer to [8], where the reader can find a large list of relevant literature on the subject.

Although a simple dichotomous process contains some essential features of the movement of motor proteins, it can on no account provide a realistic description of the ATP hydrolysis. The main problem is that, for a ratchet-like potential, the direction of the current is fixed. It is therefore interesting to study other noise processes as well. Mielke recently developed a method that applies both to Magnasco's model of a fluctuating force [9] and to the model by Astumian and Bier [10]. For a fluctuating sawtooth potential, he observed in several cases a current reversal for slightly different parameter sets of the multiplicative noise. Despite its simplicity, the model shows that small modifications of the motor protein suffice to make it move in the opposite direction. Other noise processes that can take not only two values as the dichotomous process can also be motivated from the biological situation of the motor protein. Typically, the motor protein undergoes several conformational changes, so that the interaction between the motor protein and the substrate must be described by several interaction potentials, not only two.

In this paper, we apply the method developed by Mielke to treat the movement in a fluctuating potential. Up to now, most efforts have concentrated on studying the influence of the noise parameters on the induced stationary current. Therefore calculations were performed taking the simplest asymmetric poten-

tial, a sawtooth ratchet. We rather focus on how the current varies when the geometry of the potential is changed. This question is of general interest, since one might expect new phenomena in a more complex potential. It is also of relevance for the question, whether or not these models can be used to construct a realistic picture of motor proteins. As we will show, the stationary current, which is the most important quantity to be calculated, depends essentially on the specific form of the potential. Therefore we conclude that a quantitative comparison between experimental findings and theoretical predictions from the simple model should be taken with care. A small change of the potential may change the picture quantitatively and even qualitatively.

After defining the model, we derive a set of tridiagonal recursion relations to calculate the current and the stationary probability distribution. In Section 3 we take these relations as a starting point to discuss the limiting case of white noise and compute the current up to second order in the correlation time. In Section 4 we present exact numerical results for piecewise linear potentials. It turns out that direction and rate of the movement depend strongly on the details of the potential. Section 5 summarizes the main conclusions of the present work and discusses the relevance of our results for the motion of molecular motors.

2 Definition of the model

The overdamped Brownian motion of a particle in a fluctuating periodic potential can be described by a Langevin equation,

$$\frac{dx}{dt} = -z(t)\frac{\partial V(x)}{\partial x} + \sqrt{2T}\xi(t). \quad (2.1)$$

We have chosen the units so that the friction coefficient is unity. The second term on the right hand side describes the thermal noise, as usual one has

$$\langle \xi(t) \rangle = 0 \quad \langle \xi(t)\xi(t') \rangle = \delta(t-t'). \quad (2.2)$$

The first term describes a fluctuating periodic potential. $V(x)$ is periodic with period L . We restrict ourselves to the case where the amplitude $z(t)$ of the potential $V(x)$ fluctuates. This case has also been studied by Astumian and Bier [5] and by Prost *et al.* [6]. As mentioned above, they discussed only the case where $z(t)$ takes two different values. We consider the more general case where $z(t)$ is a Markov process described by a general Fokker–Planck equation

$$\frac{\partial p(z,t)}{\partial t} = M_z p(z,t). \quad (2.3)$$

The operator M_z has one eigenvalue $\lambda_0 = 0$. The corresponding right eigenfunction $\phi_0(z)$ is the stationary distribution of the Markov process $z(t)$. The other eigenvalues are non-positive. The eigenvalue equation of M_z is

$$M_z \phi_n(z) = -\lambda_n \phi_n(z), \quad (2.4)$$

where $\phi_n(z)$ are the right eigenfunctions of M_z . We assume that $0 < \lambda_1 \leq \lambda_2 \leq \dots$. Without loss of generality we take $\langle z \rangle > 0$. The time-dependent autocorrelation function of $z(t)$ satisfies

$$\langle z(t)z(t') \rangle - \langle z \rangle^2 \propto e^{-|t-t'|/\tau} \quad (2.5)$$

for large $|t-t'|$. The correlation time τ is determined by the largest negative eigenvalue of M_z , i.e. $\tau = \lambda_1^{-1}$. We restrict ourselves to a class of processes for which

$$z\phi_n(z) = \gamma_{n,n+1}\phi_{n+1}(z) + \gamma_{n,n}\phi_n(z) + \gamma_{n,n-1}\phi_{n-1}(z), \quad n \geq 1. \quad (2.6)$$

We assume that the stationary distribution $\phi_0(z)$ of z is normalized to unity. Due to the recursion relations (2.6) the eigenfunctions $\phi_n(z)$ can be written as $\phi_n(z) = g_n(z)\phi_0(z)$ where $g_n(z)$ are orthogonal polynomials with respect to the weight function $\phi_0(z)$,

$$\int dz g_n(z) g_m(z) \phi_0(z) = \delta_{n,m}. \quad (2.7)$$

This class of Markov processes is very general. It contains many processes that occur in typical situations such as the Ornstein–Uhlenbeck process, the dichotomous process, sums of dichotomous processes, and kangaroo processes.

Having defined the stochastic process $z(t)$ via the Fokker–Planck equation (2.3) it is natural to work with a Fokker–Planck equation for the problem described by (2.1). To do this one has to introduce a joint probability density $\rho(x, z, t)$ for $x = x(t)$ and $z = z(t)$. The Fokker–Planck equation for $\rho(x, z, t)$ can be written in the form

$$\frac{\partial \rho(x, z, t)}{\partial t} = -\frac{\partial}{\partial x} \left(z f(x) - T \frac{\partial}{\partial x} \right) \rho(x, z, t) + M_z \rho(x, z, t). \quad (2.8)$$

In the following we will only consider static properties of our model. Therefore it is sufficient to calculate the static joint probability density $\rho(x, z)$. It satisfies (2.8) with vanishing left hand side. For the class of processes under consideration, it is suitable to expand $\rho(x, z)$ in the complete system of right eigenfunctions $\phi_n(z)$ of M_z ,

$$\rho(x, z) = p_0(x)\phi_0(z) + \sum_{n=1}^{\infty} (-1)^n \phi_n(z) p'_n(x). \quad (2.9)$$

Using the equations (2.6) one derives easily a set of recursion relations for $p_n(x)$.

$$J = \gamma_{0,0} f(x) p_0(x) - T p'_0(x) - \gamma_{0,1} f(x) p'_1(x), \quad (2.10)$$

$$\gamma_{0,1} f(x) p_0(x) = \lambda_1 p_1(x) + \gamma_{1,1} f(x) p'_1(x) - T p''_1(x) - \gamma_{1,2} f(x) p'_2(x), \quad (2.11)$$

$$\gamma_{n-1,n} f(x) p'_{n-1}(x) = \lambda_n p_n(x) + \gamma_{n,n} f(x) p'_n(x) - T p''_n(x) - \gamma_{n,n+1} f(x) p'_{n+1}(x) \text{ for } n > 1. \quad (2.12)$$

J is an integration constant which has a simple physical meaning, it is the static current. A slightly different derivation of these equations has been given in [9, 10]. In general it is not possible to solve these equations, but they provide a good starting point for various approximations and solutions for special cases. One possibility is to solve (2.10–2.12) using matrix continued fractions (see e.g. [11]). The continued fraction has to be truncated, it can then be evaluated numerically. Another possibility is to solve (2.10–2.12) for small τ perturbatively. This has been done to first order in [10], and higher orders can be calculated straight forward. We give the results up to second order in the next section.

In the special case where the potential $V(x)$ is piecewise linear, the force $f(x)$ is piecewise constant and (2.10–2.12) become linear equations with constant coefficients that can be solved explicitly. The remaining task is to satisfy the continuity conditions for $p_n(x)$. For the simplest case, a sawtooth potential, this has been explained in detail in [9, 10]. A generalization to other piecewise linear potentials is straight forward. In Section 4 we will present some results for a potential with three and four pieces.

3 τ -expansion

As already discussed in [10], it is useful to construct a τ -expansion for constant $\gamma_{n,m}$ in the case of a fluctuating potential. When studying a potential driven by a noisy force one often uses a τ -expansion for

fixed $D = \gamma_{0,1}^2/\tau$. In the case of a fluctuating potential, however, this would imply arbitrary large potential fluctuations, which is clearly unphysical.

The τ -expansion can be obtained using standard perturbation theory for linear operators [12]. But it is also possible to start directly from the recursion relations (2.10–2.12). To obtain a τ -expansion for constant $\gamma_{n,m}$, one uses

$$p_0(x) = p_{00}(x) + p_{01}(x)\tau + p_{02}(x)\tau^2 + O(\tau^3), \quad (3.1)$$

for $p_0(x)$ and similarly

$$J = J_0 + J_1\tau + J_2\tau^2 + O(\tau^3). \quad (3.2)$$

This ansatz implies that $p_n(x) = O(\tau^n)$. Thus the lowest order terms can be obtained from (2.10), which yields

$$p_{00}(x) = Ce^{-\frac{\gamma_{0,0}V(x)}{T}} \quad (3.3)$$

and $J_0 = 0$. C is fixed using the normalization of $p_{00}(x)$. In the next order, the term containing $p_1(x)$ in (2.10) becomes important. The equation can now be solved by means of a variation of the constant,

$$p_{01}(x) = C^{(1)}(x)e^{-\frac{\gamma_{0,0}V(x)}{T}} \quad (3.4)$$

For $C^{(1)}(x)$ we obtain

$$C^{(1)}(x) = -\frac{1}{T} \int_0^x \left(J_1 + \gamma_{0,1}^2 f(y) \left\{ \frac{d}{dy} f(y) p_{00}(y) \right\} \right) e^{\frac{\gamma_{0,0}V(y)}{T}} dy + C_0^{(1)}. \quad (3.5)$$

The constant $C_0^{(1)}$ can be fixed through $\int_0^L p_{01}(x) dx = 0$. For J_1 one obtains using $C^{(1)}(0) = C^{(1)}(L)$

$$J_1 = -\frac{\gamma_{0,1}^2}{T} \gamma_{0,0} \frac{\int_0^L f(x)^3 dx}{\int_0^L e^{-\frac{\gamma_{0,0}V(x)}{T}} dx \int_0^L e^{\frac{\gamma_{0,0}V(x)}{T}} dx}. \quad (3.6)$$

The sign of J_1 depends only on the sign of $\gamma_{0,0}f(x)$. This means that to first order in τ one never has a current reversal. Later in the discussion of our numerical results we will see that the current changes its sign as a function of τ . Therefore it is interesting to see whether this behaviour can be obtained within the τ -expansion. The calculations are straight forward, for additional details we refer to [10]. The final result for the second term J_2 is

$$\begin{aligned} J_2 = & C\tilde{C}\gamma_{0,1}^2 \left\{ (5\gamma_{0,0} - \gamma_{1,1}) \int_0^L f'(x)^2 f(x) dx + \frac{\gamma_{0,0}^2(\gamma_{1,1} - \gamma_{0,0})}{T^2} \int_0^L f(x)^5 dx \right\} \\ & + \tilde{C}\gamma_{0,1}^2 \left\{ \int_0^L C^{(1)}(x) f(x) f'(x) dx - \frac{\gamma_{0,0}}{T} \int_0^L f^3(x) C^{(1)}(x) dx \right\}, \end{aligned} \quad (3.7)$$

with $\tilde{C} = [\int_0^L \exp(\gamma_{0,0}V(x)/T) dx]^{-1}$. Depending on $\gamma_{1,1}$ and on $f(x)$ this expression may be positive or negative. This shows that for sufficiently large τ one may have a current reversal.

The τ -expansion presented here has been constructed perturbatively. The n -th order is well defined if the n -th derivative of the potential $V(x)$ exists. Thus the τ -expansion is well defined only for analytic potentials, otherwise it breaks down. This happens if we take a piecewise linear potential. In that case already J_2 is not defined. A similar observation is made in for a fluctuating force. In [13] it was shown how one can obtain an asymptotic τ -expansion for that model. In general one obtains an expansion in $\sqrt{\tau}$. But in contrast to the model with a fluctuating force, the first term J_1 in the perturbative τ -expansion calculated above is always correct in the present case.

4 Exact numerical results

As already mentioned above, the recursion relations become differential equations with constant coefficients if the force is piecewise constant. Let us divide the interval $I = [0, L]$ into a set of disjoint intervals I_k and let us assume that $f(x) = f_k$ if $x \in I_k$. An appropriate ansatz for $p_n(x)$ is

$$p_0(x) = \sum_r c_{r,k} a_{0,k}^{(r)} \alpha_k^{(r)} e^{\alpha_k^{(r)} x} + b_{0,k} \text{ if } x \in I_k, \quad (4.1)$$

$$p_n(x) = \sum_r c_{r,k} a_{n,k}^{(r)} e^{\alpha_k^{(r)} x} + b_{n,k} \text{ if } n \geq 1, x \in I_k. \quad (4.2)$$

Inserting these expression in the recursion relations one obtains a generalized eigenvalue problem for the coefficients $a_{n,k}^{(r)}$ and $\alpha_k^{(r)}$,

$$\mathbf{A}_k \vec{a}_k = \alpha_k \mathbf{B}_k \vec{a}_k + T \alpha_k^2 \vec{a}_k \quad (4.3)$$

$$\mathbf{A}_k = \begin{pmatrix} 0 & & & \\ & \lambda_1 & 0 & \\ & & \lambda_2 & \\ 0 & & & \ddots \end{pmatrix}, \quad \vec{a}_k = \begin{pmatrix} a_{0,k} \\ a_{1,k} \\ \vdots \end{pmatrix} \quad (4.4)$$

$$\mathbf{B}_k = \begin{pmatrix} \gamma_{0,0} f_k & \gamma_{0,1} f_k & & & \\ \gamma_{0,1} f_k & \gamma_{1,1} f_k & \gamma_{1,2} f_k & & 0 \\ & \gamma_{1,2} f_k & \ddots & \ddots & \\ 0 & & \ddots & \ddots & \ddots \end{pmatrix}. \quad (4.5)$$

For details of the derivation and for an analytical solution of this problem for some special noise processes, we refer to [10]. In general, one can always truncate the matrices \mathbf{A}_k and \mathbf{B}_k at some large value of n and solve the eigenvalue problem numerically. In the following we will discuss results for sums of dichotomous processes. In this case it is possible to solve the eigenvalue problem analytically. The remaining task is to calculate the coefficients $c_{r,k}$ and the current J . These quantities can be computed using the continuity of $p_n(x)$ for $n \geq 0$ and $p'_n(x)$ for $n \geq 1$ at the points where the force jumps from one value to another. These continuity conditions together with the normalization of $p_0(x)$ yield a set of linear equations for the unknown coefficients $c_{r,k}$ in the ansatz (4.1–4.2) and the current J . The current can finally be expressed as a ratio of two determinants. A detailed description of this procedure has been given in [10] for a sawtooth potential, i.e. for the case where $f(x)$ takes two values. For a single dichotomous process the current has a fixed sign, but already for a sum of two or more dichotomous processes the current may change its sign as a function of the parameters, e.g. of τ . The main motivation of the present work was to study the dependence of the current as a function of the potential. The simplest case is that of a force $f(x)$ that takes three instead of two different values, i.e.

$$f(x) = \begin{cases} f_1 & \text{if } x \in I_1 = [0, L_1) \\ f_2 & \text{if } x \in I_2 = [L_1, L_2) \\ f_3 & \text{if } x \in I_3 = [L_2, L) \end{cases}. \quad (4.6)$$

The parameters cannot be chosen independently. Using $L_0=0, L_3=L$ and introducing the interval lengths $\Delta_k := L_k - L_{k-1}$, we have $\sum_{k=1}^3 f_k \Delta_k = 0$ due to the periodicity of $V(x)$. When the potential is close to a simple sawtooth potential, for example if f_1 and f_2 are negative, f_3 is positive and Δ_3 is smaller than $\Delta_1 + \Delta_2$ one observes a behaviour that is similar to what has been obtained in [10]. But if $\Delta_1 + \Delta_2$ is

close to Δ_3 new phenomena can be observed. If $\Delta_1 + \Delta_2 = \Delta_3$ and $f_1 = f_2$, the potential has inversion symmetry and consequently $J = 0$. In the following our goal will be to study what happens if one has a small deviation of the inversion symmetric case. For instance one can take a situation where Δ_1 is much smaller than Δ_2 and $|f_1|$ is much larger than $|f_2|$. A typical form of the potential is shown in Figure 1. We begin with the discussion of the behaviour of the system if $z(t)$ is a simple dichotomous process

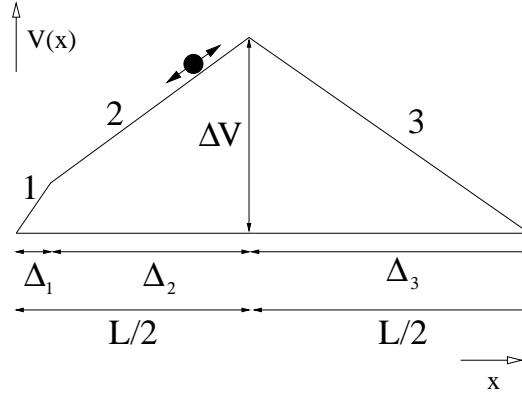


Figure 1: A slight symmetry broken three piece linear potential.

that takes two values z_1 and z_2 with equal probability. We will always assume that $\langle z \rangle = \gamma_{0,0} > 0$, i.e. $z_1 + z_2 > 0$. Then the first term in the τ -expansion yields a positive current. It turns out that, depending on the special choice of the parameters, one obtains a current reversal even in the case of a dichotomous noise process. An example is shown in Figure 2. Here we have $z_1 = 0$ and $z_2 > 0$. Let us first assume that τ is small. If $z = z_1$, the particle is only subject to thermal fluctuations. When the potential switches to z_2 , the probability to find the particle on the longest potential slope 3 is the same than to find it on any of the two other slopes. For not too large temperatures, the thermal perturbation in the equation of motion can be neglected. A simple calculation then shows that the time required to reach the minimum of the potential along two potential slopes is minimized if the slopes are equal. On average the particle moves to the right; as predicted by the τ -expansion, a positive current flows. We now consider the opposite situation of sufficiently large τ . Then one has a nearly adiabatic behaviour. But, as shown in [10], the current vanishes in the adiabatic limit. The first correction is of order $O(1/\tau)$. Suppose that the temperature is not too large. If $z = z_2$, the particle will move towards the minimum of the potential and we can assume that it reaches a nearly static probability distribution $\propto \exp(-zV(x)/T)$. This distribution is peaked near the minimum, but due to the asymmetry of the potential the probability to find the particle on the left hand side of the minimum will be larger than to find it on the right hand side. When z switches to $z_1 = 0$, the particle moves only due to the thermal noise. But since the initial probability distribution is asymmetric, the probability distribution at a finite time will be asymmetric as well. It is simply given by the convolution of the initial distribution with a Gaussian. Therefore, when z switches back to $z = z_2$, the probability to reach the next minimum on the left hand side will be larger than to reach the next minimum on the right hand side. This produces a net current to the left. Therefore the model shows a current reversal. This can be observed in Figure 2. For small values of the interval length $\Delta_1 = L_1$, the region where the current is positive is very small, for larger values of L_1 the region where the current is negative

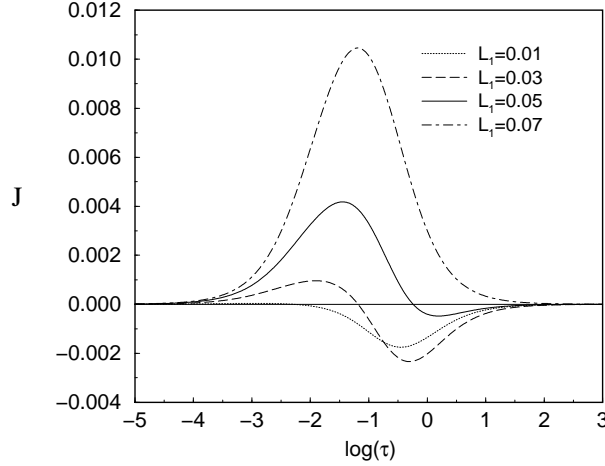


Figure 2: The current as a function of $\log(\tau)$ for different potentials. The parameters of the noise are $N = 1$, $z_1 = 0$ and, $z_2 = 2$. The temperature is $T = 0.04$. Each potential has the common parameters $L_2 = 0.5$, $L_3 = 1$, $f_1 = -2$, $f_3 = 0.47$ and different values of the interval length $\Delta_1 = L_1$ and the slope f_2 . The corresponding values of f_2 are: $L_1 = 0.01 \rightarrow f_2 \approx -0.439$; $L_1 = 0.03 \rightarrow f_2 \approx -0.372$; $L_1 = 0.05 \rightarrow f_2 \approx -0.3$; $L_1 = 0.07 \rightarrow f_2 \approx -0.221$.

reduces rapidly.

It is interesting to study what happens when one varies other parameters of the system, e.g. the temperature, or what happens for a more general noise process, which showed already a current reversal in the case of a sawtooth potential. In the following we present some typical results for a potential with the parameters $f_1 = -2$, $f_3 = 0.47$, $L_1 = 0.03$, $L_2 = 0.5$, and $L = 1$. From these values one obtains $f_2 \approx -0.372$ and $\Delta V = |f_3 \Delta_3| = 0.235$. We have chosen these parameters since, as seen in Figure 2, they show the new current reversal very clearly, whereas for somewhat larger or smaller values of L_1 the regions where the current is negative or positive becomes very small.

Let us first discuss the current as a function of the temperature for a single dichotomous process. In Figure 3 we show results for the current as a function of $\log(\tau)$ for various temperatures. The dichotomous process takes the two values $z_1 = -0.3$ and $z_2 = 2.3$. One observes that for a small temperature region around $T = 0.027$ the current is positive for small τ , becomes negative when τ increases and then becomes positive again. The third region is strongly enhanced when the temperature is smaller and it vanishes when the temperature becomes larger. To understand this new effect, we first consider the system at temperatures, for which the condition $z_1^2 \max(f(x))^2 \lesssim 2T \ll z_2^2 \min(f(x))^2$ holds. Then one basically has the same situation as in the case where one of the coupling constants is zero and the other positive. When $z(t) = z_1$, the motion of the particle in the potential is smeared out by the thermal noise. If we now slowly turn the temperature down, the particle will begin to feel the influence of the flat potential. Let us consider the nearly adiabatic case at sufficiently low temperatures. If $z(t) = z_2$, the particle reaches a nearly stationary probability distribution. When the potential switches to z_1 , the distribution spreads out and the particle diffuses over several potential valleys. Since the potential slopes are now much flatter, the particle has not enough time to reach the stationary distribution before the potential fluctuates and we can by no means invoke the stationarity argument used above. Nevertheless, the dynamics is again determined by the geometry of the potential: Due to the steep slope 1, the particle surmounts the right slope 3 more easily than the other two ones (see Fig. 1). On average, one obtains a positive flow.

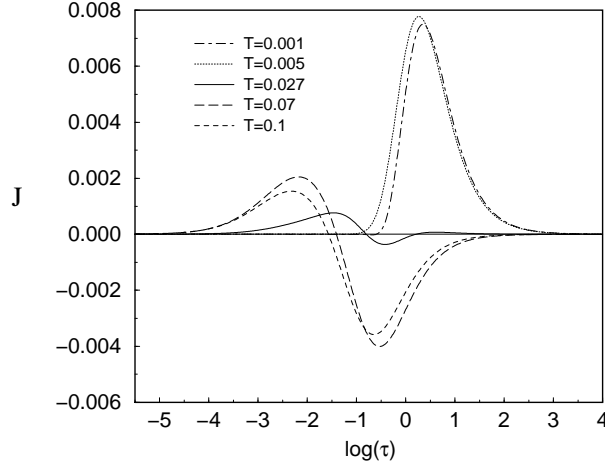


Figure 3: The current as a function of $\log(\tau)$ for a symmetric dichotomous process. The two values are $z_1 = -0.3$ and $z_2 = 2.3$.

Instead of a single dichotomous process we now take a sum of $N - 1$ identical dichotomous processes, each again with the two values z_1 and z_2 . The static distribution of z is given by

$$\phi_0(z) = \frac{1}{2^N} \sum_{k=0}^N \binom{N}{k} \delta(z - (N-k)z_1 - kz_2). \quad (4.7)$$

and we have $z_{1,2} = \frac{\langle z \rangle}{N} \pm \gamma$, where $\gamma^2 = \frac{\langle z^2 \rangle - \langle z \rangle^2}{N}$. After performing the rescaling $\gamma \rightarrow \frac{\gamma}{\sqrt{N}}$, the coefficients $\gamma_{n,m}$ are given by

$$\gamma_{n,n+1}^2 = \frac{(n+1)(N-n)}{N} \gamma^2, \quad \gamma_{n,n} = \langle z \rangle. \quad (4.8)$$

In [10] it was shown that for this class of processes the eigenvalue problem (4.3) can be solved analytically.

The question is now whether the effect observed for a single dichotomous process can be observed in this case as well, and if perhaps additional new effects occur. Next we present some results for a sum of two dichotomous processes. Let us first discuss the behaviour for large values of τ . As in the case of a single dichotomous process we have a nearly adiabatic behaviour. But now, z takes three values $2z_1$, $z_1 + z_2$, and $2z_2$. For $z_1 < 0$, $z_1 + z_2 > 0$ and small temperature the behaviour should be that of a single dichotomous process that takes the two values $2z_1$, and $z_1 + z_2$. Therefore, the sign of the current depends on the difference of z_1 and z_2 , i.e. on γ . If the condition $|2z_1| < z_1 + z_2$ holds, i.e. if $\gamma < \sqrt{2} \langle z \rangle$, it will be positive and otherwise, negative. Figures 4 and 5 confirm this qualitative discussion.

At higher temperatures, the motion in the potential $2z_1 V(x)$ is smeared out and the system behaves again as in the case of a simple dichotomous process with $z_1 = 0$ and $z_2 > 0$. From our discussion, we expect only one current reversal for all $\gamma > \sqrt{2} \langle z \rangle$. However, it turns out that for higher values of γ and sufficiently large temperatures a weak positive current is observed when τ becomes large (Figure 6). To understand the different behaviour in Figure. 5 and 6, first note that for $\gamma = 1.7$ the quantities $|2z_1| = 1.4$ and $z_1 + z_2 = 1$ have a similar numerical value, whereas for $\gamma = 2.5$ one has $2z_1 \approx -3.4$ and $z_1 + z_2 = 1$. In the first case the motion for both values $z(t)$ is determined mainly by the thermal noise when T rises; but in the second, only the motion in the potential that corresponds to the value $z(t) = \langle z \rangle$ will be smoothed out while the motion in the potentials for the other two values is not influenced so much by the thermal

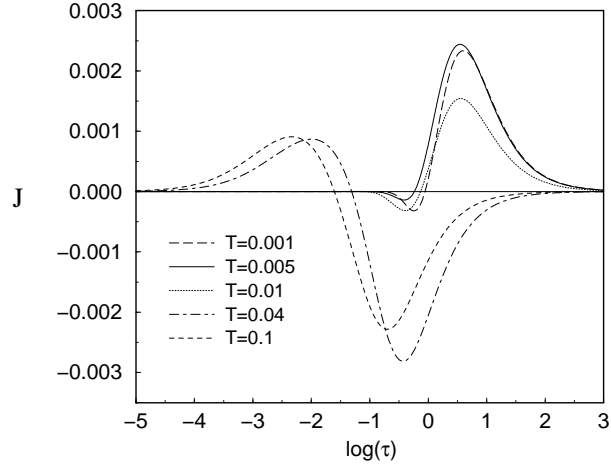


Figure 4: The current as a function of $\log(\tau)$ for a sum of two dichotomous processes at different temperatures. The average of the coupling constant and the noise strength are $\langle z \rangle = 1$ and $\gamma = 1$.

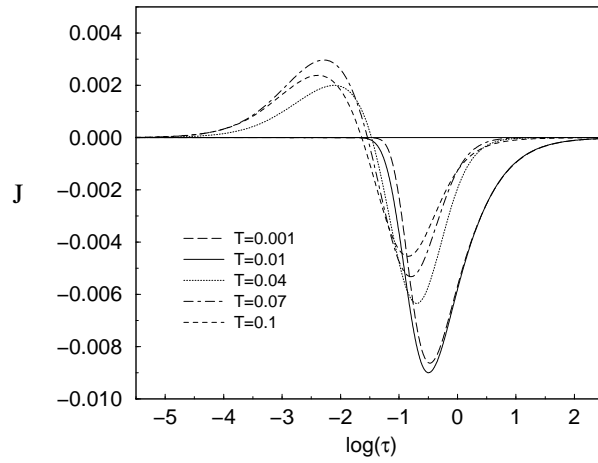


Figure 5: The current as a function of $\log(\tau)$ for a sum of two dichotomous processes at different temperatures. The parameters of the noise are $\langle z \rangle = 1$ and $\gamma = 1.7$.

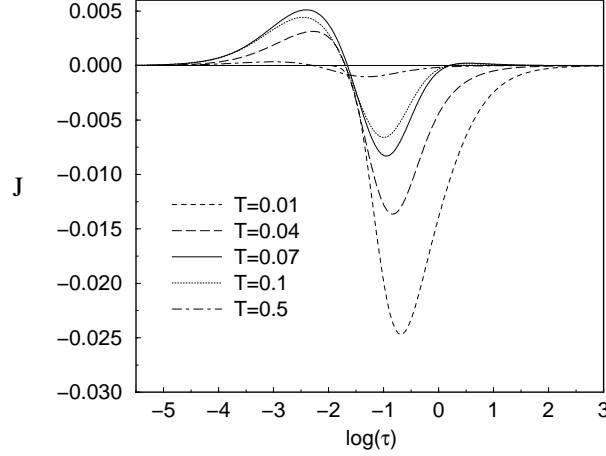


Figure 6: The current as a function of $\log(\tau)$ for a sum of two dichotomous processes at different temperatures. Here we have set $\langle z \rangle = 1$ and $\gamma = 2.5$.

noise. For large τ and not too high temperatures only the values with small $|z(t)|$ are relevant, i.e. $2z_1$ and $z_1 + z_2$. Thus the system behaves as in the case of a single process where one of the coupling constants is zero and the other is negative. This yields a small positive current.

Let us briefly discuss the behaviour of the current for a sum of N identical symmetric dichotomous processes. Figure 7 shows some plots of the current as a function of τ for different values of N . For

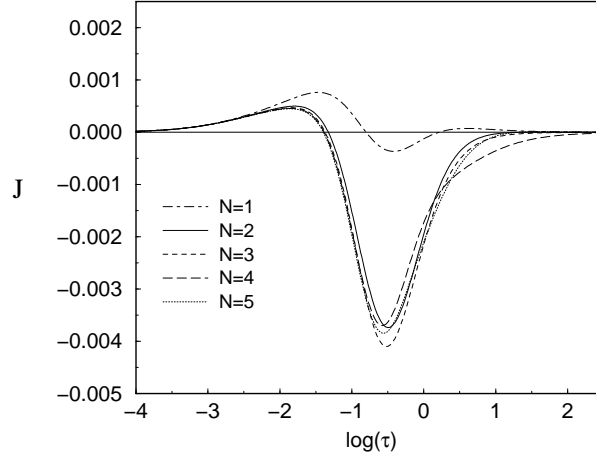


Figure 7: The current as a function of $\log(\tau)$ for a sum of dichotomous processes. N takes the values 1,2,3,4 and 5. The other parameters of the noise read $\langle z \rangle = 1$ and $\gamma = 1.3$; the temperature is $T = 0.027$.

small values of the correlation time ($< 10^{-2}$), all curves merge into a single curve. This is a generic feature, which holds also for general potentials $V(x)$. The reason is that, according to (3.6) and (3.7), the coefficients J_1 and J_2 of the τ -expansion are the same for all N , since the quantities $\gamma_{0,0}$, $\gamma_{0,1}$ and $\gamma_{1,1}$ do not depend on N . In contrast, the behaviour of each curve is different near the adiabatic limit; for $N > 1$, the effect responsible for a positive current disappears.

The fact that all plots lie so close to each other suggests that they rapidly converge to a single curve for $N \rightarrow \infty$. In this limit, the sum of dichotomous processes yields a well known Gaussian process, the so-called Ornstein–Uhlenbeck process [14]. In this case the potential, rather than jumping between different states, suffers a continuous distortion. One therefore expects that some mechanisms that lead to a current reversal cancel. Nevertheless, our results show that the current changes its sign once, in contrast to the case of a sawtooth potential, where the sign of the current is fixed [10]. This behaviour is also predicted by the τ -expansion, which leads to a current reversal for potentials of the form discussed above and an Ornstein–Uhlenbeck process.

The validity of the expansion around the white noise limit can be tested with the help of the exact numerical results. In Figure 8 two exact plots of the current for $N = 1$ and $N = 2$ and the first order term

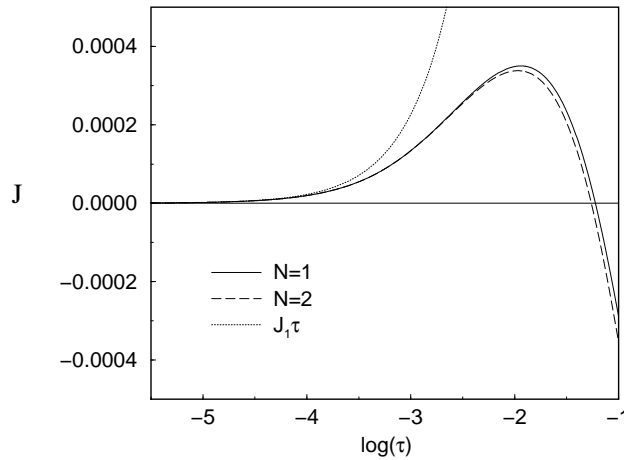


Figure 8: Two plots of the current as a function of $\log(\tau)$ computed for a simple dichotomous process (solid line) and a sum of two processes (dashed line) are shown together with the first order term (dotted line) of the τ -expansion. Here we have set $\langle z \rangle = 1$ and $\gamma = 0.6$. The temperature is $T = 0.04$.

of the τ expansion are depicted. The quantitative agreement with the exact curves is remarkably good for values of τ below 10^{-4} .

To conclude this section let us discuss briefly what happens for more complicated potentials. It is straight forward to do the same calculations as above for e.g. a piecewise linear potential with four (or more) pieces. We have done several calculations for a potential with four pieces. The results for small and large values of τ are similar to the results reported for the potential with three pieces. For small τ a current reversal may occur and can be predicted by the τ -expansion. For large τ , in the nearly adiabatic limit, the current is positive or negative, depending on the temperature and the noise parameters. The mechanism we discussed in that case for the potential with three pieces can be carried over to the more general case. For intermediate values of τ , the current shows a more complicated behaviour. Depending on T and γ , one observes additional minima and maxima for J as a function of τ . On the other hand, we never observed more than two current reversals for J as a function of τ .

5 Conclusions

The main result of this paper is that a new kind of current reversal occurs for a Brownian particle in a fluctuating potential, if the potential is not a simple sawtooth potential. For a saw-tooth potential a current reversal has only been observed for more complicated noise processes, but not for a simple dichotomous

process or for the Ornstein–Uhlenbeck process [5, 6, 10]. In a more complicated potential a current reversal even occurs for the dichotomous process and the Ornstein–Uhlenbeck process. It can even be predicted by a simple τ -expansion carried out to second order. For a general potential we have derived the first two non-vanishing terms of the expansion around the white noise limit and we have shown that, depending on the noise parameters and the shape of the potential, they may have different signs, thus leading to a current reversal.

The stationary current depends strongly both on the statistics of the coloured fluctuations and the details of the potential. Depending on the range of τ and T , the current has a different direction and magnitude.

We have focused on the special case of a piecewise linear potential. Our numerical results show that small deviations of the inversion symmetric case change the qualitative behaviour of the system dramatically. If one takes for instance a slight asymmetric three piece linear potential, the current may change its sign as a function of τ more than once, even in the case of a simple dichotomous process. The number of current reversals depends on the relative sign of the coupling constants z_1 and z_2 : If both are positive or one is positive and the other one is zero, only one current reversal is observed, whereas in the case $z_1 < 0$ and $z_1 + z_2 > 0$ a new low temperature effect takes place and provokes an additional current reversal for large τ . In this situation, the induced current tends to a finite value when $T \rightarrow 0$.

Depending on the time scale of the fluctuations, the asymmetry of the potential acts on the particle in a different way: In the nearly adiabatic limit, the thermally driven particle surmounts one of the adjacent potential barriers more easily than the other one, whereas for small τ (and not too high temperatures), the different drift times down the three potential slopes favour one direction of movement. Both effects are purely dynamical, it is not possible to explain the behaviour using transition rates calculated in the adiabatic limit.

For a sum of two dichotomous processes, the system may be described by an effective dichotomous process if τ is sufficiently large. The behaviour depends on the sign of the average of the coupling constant for the effective process, i.e. on $\langle z \rangle$ and γ . When T rises, some values of $z(t)$ will be washed out by the thermal noise. Therefore, the choice of the coupling constants of the effective process depends on temperature.

In the general case of a sum of N dichotomous processes, we have seen that the current does not depend on the noise details for sufficiently small τ . Whereas in the case of a sawtooth potential the current changes sign only if N is odd [10], for a proper form of the three piece potential one observes at least one current reversal for all values of N .

Since our numerical results have been obtained only for a piecewise linear potential, we would like to emphasize that our results hold for general potentials as well. As mentioned above the current reversal in the case of a dichotomous process or in the case of the Ornstein–Uhlenbeck process can be predicted by a second order τ -expansion for any given potential. Furthermore, the argument that for large τ the behaviour of the system can be described by an effective dichotomous process, is true for a general potential as well.

Let us discuss the relevance of our results for the motion of molecular motors. In [10] it was argued that the basic features of the movement can be described by a sum of $N - 1$ dichotomous processes, where $N \geq 3$ is the number of conformational changes of the motor protein. Even if one takes a simple sawtooth ratchet as interaction potential, this model leads to a current reversal for a proper choice of the parameters. According to Astumian and Bier this means that, after redimensionalizing the equation of motion (2.1), two proteins with a slight different geometry —and thus different friction coefficients— may drift in opposite directions [15].

On the other hand, our results emphasize that rate and direction of the movement are very sensitive to the details of the potential. They suggest that slight modifications of the binding energy profile which the motor protein feels when it walks on the periodic polymer may change its direction of movement. Even

though the polymer tracks are much more symmetry broken than the potentials that we have investigated, it should be clear that a sawtooth ratchet is a too rough approximation for the actual interaction potential. Due to our results, one would expect that a small deviation of the simple sawtooth ratchet has a large effect on the current, especially in the region of intermediate τ . Therefore one should be careful: A quantitative agreement between calculated currents and experimental findings may be accidental. But the qualitative aspect of the model may be correct.

Clearly, the model is too simple to provide a realistic description of the situation in a cell. The kinetics of the ATP hydrolysis in the cell is very sensitive to temperature changes of the system. For this reason, τ and T cannot be chosen independently. Another serious difficulty is that the forces exerted by the protein on the track during the ATP hydrolysis change not only the barrier heights but also the shape of the interaction potential. This conformational flexibility is not taken into account in the model, where the interval lengths Δ_i and the relative heights of the potential teeth are time independent. But a more realistic model will contain many free parameters and, as we have shown, the results may depend strongly on each of these parameters. Therefore a more detailed experimental knowledge of the system is required.

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